

# **AUTOMATIC IDENTIFICATION OF COMPOUNDS IN A SAMPLE MIXTURE BY MEANS OF NMR SPECTROSCOPY**

## **ABSTRACT OF THE DISCLOSURE**

A process for quantitative and qualitative analysis for identifying compounds  
5 in a sample mixture involves the identification of a set of reference spectra selected according  
to a measured condition of the sample, which collectively define a composite spectrum which  
best matches a spectrum produced from the sample. The compounds associated with  
respective reference spectra of the identified set are the compounds that are determined to be  
likely to be present in the sample. Quantities of the compounds may be determined from the  
10 intensities of certain representative peaks associated with the compounds, relative to the  
intensity of a peak associated with a reference compound which is unaffected by the  
measured condition of the sample. A measured condition may be pH of the sample, for  
example, and an accurate measurement of pH can be obtained from the test spectrum. Thus,  
given a test spectrum of a sample and given a set of reference spectra, the process can  
15 identify and quantify compounds present in the sample. A process for producing reference  
spectra as a function of condition factor is also disclosed and a process for automatically pre-  
processing a spectrum from an NMR system is disclosed.

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